A self-consistent treatment of damped motion for stable and unstable collective modes*

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Abstract

We address the dynamics of damped collective modes in terms of first and second moments. The modes are introduced in a self-consistent fashion with the help of a suitable application of linear response theory. Quantum effects in the fluctuations are governed by diffusion coefficients $D_{\mu\nu}$. The latter are obtained through a fluctuation dissipation theorem generalized to allow for a treatment of unstable modes. Numerical evaluations of the $D_{\mu\nu}$ are presented. We discuss briefly how this picture may be used to describe global motion within a locally harmonic approximation. Relations to other methods are discussed, like "dissipative tunneling", RPA at finite temperature and generalizations of the "Static Path Approximation".

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*Dedicated to Professor Richard Lemmer on the occasion of his 65th birthday

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1 Introduction

The interplay of dissipation and quantum effects has been a long standing challenge to transport theory, in particular the question of the influence of damping on quantum tunneling. Convincing answers have only be found in the 80'ies by clarifying demanding problems of principal nature with the help of functional integrals, see e.g. [1] - [5]. In these approaches one first derives effective actions for global motion from which one may then deduce expressions for the decay rate of a meta-stable state. In contrast to this procedure, we like to look at the problem from the point of view of transport equations such as the one of Kramers [6] but extended to include quantum effects. By its very nature, such a transport equation reflects local properties of collective motion as displayed through the propagation in collective phase space. In the following we like to concentrate on situations where damping cannot simply be treated perturbatively. For the case of stable modes, suggestions of possible quantal equations have been made for instance in [7] and [8]. The possibility of generalizing to unstable modes has first been described in [9].

Different to those papers mentioned previously which deal with dissipative tunneling and which exploit functional integrals, we like to base our analysis on systems where collective variables are introduced *self-consistently*. For Hamiltonian dynamics, this implies that in the Hamiltonian

$$\mathcal{H} = H_{\rm intr} + H_{\rm coupl} + H_{\rm coll} \tag{1}$$

for the total system both the "collective" part $H_{\rm coll}$ as well as the coupling term are bound to be functionals of the dynamical variables of the intrinsic system. One prime example is the electron gas for which D. Bohm and D. Pines have been able to deduce such a Hamiltonian in [10]. Another example is nuclear collective motion for which an adapted version of the Bohm-Pines method can be found in [11], see also [12]. Although later on we are going to concentrate on systems for which such a Hamiltonian (1) exists it may be mentioned that our method of accounting for self-consistency in the fluctuating force can be generalized to other cases, the most prominent example being a situation in which the dynamics is described by the Landau-Vlasov equation with (collision term) (see [13]). For stable modes this method may in some sense be considered a generalization of the suggestion made by Landau [14] (see [15]).

Evidently problems like the motion from a meta-stable minimum across a potential barrier are manifestly non-linear in at least one of the collective degrees of freedom. Moreover, there are systems for which the intrinsic sub-system and its coupling to the collective part change along the dynamical path, thus prohibiting to linearize this coupling in the bath variables. In such a situation, as it is given for example in nuclear fission, the technique of functional integration is not useful anymore as the internal degrees of freedom can no longer be integrated out. It has been argued that it might be possible to handle such systems by a *locally harmonic approximation (LHA)* (see e.g. [16], [17], [12]). In this method it is not necessary to restrict the dynamics of the internal degrees of freedom to a system of (perturbed) oscillators. Certainly, as an essential intermediate step, there will appear the dynamics in linearized version for

the *collective degrees of freedom*. As already demonstrated by Kramers, in lucky cases it may even suffice to have information on the dynamics at the potential minimum and at the barrier, the latter mode being unstable. In this paper we shall address specifically these problems and study the influence of dissipation on average motion as well as on the dynamics of the second moments (fluctuations). This will be achieved within the framework of linear response theory. The latter does not only allow one to treat average motion (in a linearized fashion), it opens an ideal playground for deducing the diffusion coefficients which govern the dynamics of the second moments. To be able to treat instabilities as well, it will turn out necessary to perform suitable analytical continuations. Manipulations of the kind which will be needed here have been used before in [18], [19], but, as mentioned, not in connection with a transport equation and, hence, diffusion coefficients. As we shall see the numerical computations of these coefficients will very naturally hint to limits of the LHA at smaller temperatures.

2 Brief review of average motion

In this paper we would like ourselves to restrict to a situation in which the dynamics of interest can be described by the one quantity $\hat{F}$. For average motion this means looking at the time evolution of the expectation value $\langle \hat{F} \rangle_t$. To start with a simple situation let us suppose we are given a Hamiltonian of the type

$$\hat{H}^{(2)} = \hat{H}_0 + \frac{k}{2} \hat{F} \hat{F} \tag{2}$$

with some coupling constant k, without bothering for the moment how it has come about. Later on we are going to describe how this form may derived from more general considerations and how the k may be deduced from static properties of the system, in which case it will depend on the actual state of the intrinsic system. Let us suppose further that we are interested in harmonic vibrations. As may be well known, their frequencies and strengths can be deduced from the following response function

$$\chi_{\rm coll}(\omega) = \frac{\chi(\omega)}{1 + k\chi(\omega)} \tag{3}$$

obeying the following definition

$$\delta \langle \hat{F} \rangle_\omega = -\chi_{\rm coll}(\omega) f_{\rm ext}(\omega) \tag{4}$$

The $\delta \langle \hat{F} \rangle_\omega$ measures the Fourier transform of the deviation of $\langle \hat{F} \rangle_t$ from the equilibrium value $\langle \hat{F} \rangle_0$, as it follows from the response of the system in linear order to an external field $f_{\rm ext}(\omega)$, with the coupling being given by $\delta \hat{H} = f_{\rm ext} \hat{F}$. The $\chi(\omega)$ is the Fourier transform of the response function defined by

$$\widetilde{\chi}(t-s) = \Theta(t-s) \frac{i}{\hbar} {\rm tr} \left(\hat{\rho}^0_{\rm qs} \left[\hat{F}^I(t), \hat{F}^I(s) \right] \right) \tag{5}$$

with the $\hat{\rho}^0_{\rm qs}$ representing the equilibrium density operator associated to the Hamiltonian $\hat{H}_0$. Notice please that this function is governed entirely by *intrinsic* properties, different to the $\chi_{\rm coll}(\omega)$ which contains information on collective motion.

We should expect average dynamics to be closely related to the mean field approximation. Indeed, for the latter one readily verifies the following Hamiltonian

$$\hat{H}^{(2)}_{\rm mf} = \hat{H}_0 + (Q - Q_0)\hat{F} \tag{6}$$

where the abbreviation

$$k\langle\hat{F}\rangle_t = Q - Q_0 \tag{7}$$

has been used. One may now simply apply the Clausius-Mosotti construction to derive the form (3) from (4) and (7).

For the following it will show convenient to add to the Hamiltonian $\hat{H}^{(2)}_{\rm mf}$ of (6) a c-number term and thus to introduce a $\hat{H}(\hat{x}_i, \hat{p}_i, Q)$ like

$$\hat{H}(\hat{x}_i, \hat{p}_i, Q) = \hat{H}(\hat{x}_i, \hat{p}_i, Q_0) + (Q - Q_0)\hat{F}(\hat{x}_i, \hat{p}_i, Q_0) + \frac{1}{2}(Q - Q_0)^2 \langle\frac{\partial^2 \hat{H}(\hat{x}_i, \hat{p}_i, Q)}{\partial Q^2}\rangle_{Q_0}. \tag{8}$$

Identifying $\hat{H}(\hat{x}_i, \hat{p}_i, Q_0) = \hat{H}_0$ and the expectation value on the very right with

$$-k^{-1} = \langle\frac{\partial^2 \hat{H}(\hat{x}_i, \hat{p}_i, Q)}{\partial Q^2}\rangle_{Q_0} \tag{9}$$

one sees that the total energy of the system $E_{\rm tot} = \langle\hat{H}^{(2)}_{\rm mf}\rangle - \frac{k}{2}\langle\hat{F}\rangle\langle\hat{F}\rangle$ can simply be expressed as the expectation value $\langle\hat{H}(\hat{x}_i, \hat{p}_i, Q)\rangle$ of the one-body Hamiltonian $\hat{H}(\hat{x}_i, \hat{p}_i, Q)$.

This discussion has demonstrated the intimate relation between a Hamiltonian of the form (8) and the one of (2) involving a schematic two-body interaction. On the level of the mean field approximation the latter becomes equivalent to the former. However, the $\hat{H}^{(2)}$ of (2) allows one to treat fluctuations in $\hat{F}$, or what will turn out more convenient in $Q - Q_0$, about its average value. Indeed, later on we will be exploiting exactly this feature when we are going to quantize the "collective variable" Q. Conversely, as often mean field approximations are more easily accessible numerically than solutions of the full Schrödinger or Heisenberg equations (of the many body problem), one may start from such a $\hat{H}(\hat{x}_i, \hat{p}_i, Q)$ and construct the effective two body interaction appearing in $\hat{H}^{(2)}$.

A prominent example from nuclear physics is given when one tries to simulate the mean field approximation via the deformed shell model. In that case the Q is introduced as a c-number variable specifying the shape of the nucleus. The latter then appears both in the single particle potential as well as in the liquid drop energy. To account for the latter is necessary because otherwise one would not be able to calculate reliably the total energy of the system. This can be done with the help of the Strutinsky renormalization. How one may then proceed to construct a Hamiltonian of the type $\hat{H}(\hat{x}_i, \hat{p}_i, Q)$ has been worked out in detail in [20].

It is more than conceivable that one might start from even more microscopic theories like the one of Hartree-Fock involving effective forces or the Relativistic Mean Field theory. An

equation like (7) would then appear as a constraint for possible variations in the deformation of the self-consistent field. After appropriate linearizations and after applying time dependent perturbation theory in suitable manor one would end up in a form like (3), provided that one is interested in the change of the expectation value of the same operator $\hat{F}$ which specifies the variation in the density. In general the response "function" would have tensor character, of course.

In this context one may mention examples worked out for Landau Fermi liquid theory in [21], [13]. Looking at general modes of the single particle density in phase space for the associated response functions $\chi_{\rm coll}(\omega)$ forms similar to the one given in (3) have been deduced. There it might only happen that the "coupling constant" k may depend on the wave vectors of the various modes.

2.1 Extension to finite excitations and large scale motion

In the following we would like to concentrate on the example for which a Hamiltonian $\hat{H}(\hat{x}_i, \hat{p}_i, Q)$ is given, which depends parametrically on a c-number $Q(t)$ representing the collective degree of freedom. It is this example which is developed farthest theoretically and which still can be handled numerically even for such complex situations as nuclear fission [22], [23]. As described in various papers (see e.g. [24] and [12], in particular), with such a Hamiltonian it is possible to derive an intrinsically consistent theory for collective motion of large scale provided there is a clear separation of time scales.

Let $\tau_{\rm coll}$ be a relevant measure for a collective time scale and τ the one for the remaining degrees of freedom, henceforth called the intrinsic ones. For time lapses δt with $\tau \leq \delta t \ll \tau_{\rm coll}$ one may describe collective motion within a (locally) harmonic approximation. This is achieved by exploiting the expansion (8) and identifying simultaneously the unperturbed density operator $\hat{\rho}^0_{\rm qs}$ as the one corresponding to the Hamiltonian $\hat{H}(\hat{x}_i, \hat{p}_i, Q_0)$. This density operator may then either be a function of temperature or entropy depending which distribution we want to use for parameterizing the equilibrium. For the sake of simplicity, in this paper we will choose the canonical one later on, but we may refer to [12] for a discussion of the more general case. Thus we may write for the density $\hat{\rho}^0_{\rm qs} = \hat{\rho}_{\rm qs}(Q_0, T_0)$, with the Q_0 and the T_0 to represent those values which the "macroscopic" variables Q, T have during the time interval δt.

As shown in [24] and [12] all the steps discussed above for the genuinely harmonic case may then be taken over. We must expect, of course, that all quantities will depend on the actual quasi-static state of the system which is being specified by the pair of variables Q_0, T_0. This is true in particular for the coupling constant k which can be written in the form

$$-k^{-1} = \left.\frac{\partial^2 E(Q, S_0)}{\partial Q^2}\right|_{Q_0} + \chi(0) \equiv C(0) + \chi(0)\,. \tag{10}$$

Here $E(Q, S_0)$ is meant to represent the internal energy of the system, with the entropy S_0 being understood to be calculated for given Q_0, T_0. (It is possible, of course, to rewrite this formula in terms of derivatives of the free energy). The $\chi(0)$ stands for the static response and

the $C(0)$ is introduced as a short hand notation for the local static stiffness. To derive this relation, together with the form (3) for the collective response function, one needs to apply similar arguments as mentioned before but has to care for possible changes in the quasi-static properties of the system. In doing so one may be guided by the fact that within the harmonic approximation (for the motion in Q) entropy can be assumed to be constant (to leading order), as it will change with velocity only quadratically. Using this hypothesis, in formal sense the derivation of the form of the collective response $\chi_{\rm coll}(\omega)$ follows identically the one given above and which ended in (3), provided the adiabatic susceptibility $\chi^{\rm ad}$ is identical to the static response, $\chi^{\rm ad} = \chi(0)$; for a general discussion of the relevance of this property see [25] and [12].

The existence of equilibrium for the nucleonic degrees of freedom requires the presence of residual interactions. However, it would be beyond the scope of any realistic theory to allow for both a detailed treatment of such interactions as well as numerical applications, say for a calculation of the transport coefficients which such a theory aims at. It has been suggested, therefore, to acount for that by dressing the particles and holes (of the deformed shell model) by a self energy whose imaginary part is given by

$$\Gamma(\omega, T) = \frac{1}{\Gamma_0} \, \frac{(\hbar\omega - \mu)^2 + \pi^2 T^2}{1 + \frac{1}{c^2}\left[(\hbar\omega - \mu)^2 + \pi^2 T^2\right]} \,, \tag{11}$$

with μ being the chemical potential. It is this imaginary part which finally will be responsible for the presence of macroscopic damping. It would out of scope of the present paper to explain more details; instead, the reader is referred to [12]. In numerical applications the following values have been used for the two parameters: $\Gamma_0 = 33MeV$ and $c = 20MeV$.

With respect to the choice of Q_0, we should like to note that for the general situation away from the potential minimum, the Q_0 in (7) is to be replaced by the center Q_m of the oscillator approximating the "true" static energy $E(Q, S_0)$ in the neighborhood of the Q_0 of (8) (see e.g.[12]). Furthermore, we want to mention that the discussion to come shall be restricted to situations of negative coupling constants, which for the case of an instability will imply the $\mid C(0) \mid$ to be smaller than $\chi(0)$, see below. Looking back to the two body interaction introduced in (2) this is to say that we like to restrict ourselves to effective forces being attractive. For the nuclear case this is known to correspond to motion with neutrons and protons in phase.

2.2 Reduction to single modes

The poles of $\chi_{\rm coll}(\omega)$ define possible excitations of the system, more precisely those which involve dynamics in the quantity $\langle \hat{F} \rangle$ and which are caused by that perturbation $\delta \hat{H}$ which is proportional to the $\hat{F}$ itself. Considering all of them would in the end imply strict non-Markovian behavior in $\langle \hat{F} \rangle_t$. Eventually the strength distribution is dominated by only one mode, in which case the $\chi_{\rm coll}(\omega)$ may be replaced by the response function of the damped oscillator

$$\chi^F_{\rm osc}(\omega) = -\frac{1}{M^F} \frac{1}{\omega^2 + i\omega\Gamma - \varpi^2} \tag{12}$$

with $M^F\Gamma = \gamma^F$ and $M^F\varpi^2 = C^F$, where γ^F, M^F and C^F stand for the coefficients of friction, inertia and stiffness for the (local) motion in $\delta\langle\hat{F}\rangle_t$, a feature which is easily verified from (4). For several reasons it may be advantageous to introduce the coordinate $q(t) = Q(t) - Q_m$ for which the local equation of motion writes

$$M\ddot{q}(t) + \gamma\dot{q}(t) + Cq(t) = -q_{\rm ext}(t) \tag{13}$$

This transformation is readily performed considering (7), with the Q_0 being replaced by Q_m, of course. It implies to work with the qq-response function

$$k^2\chi_{\rm coll}(\omega) = \chi_{qq}(\omega) = \left.\frac{\delta q(\omega)}{\delta(-q_{\rm ext}(\omega)}\right|_{q_{\rm ext}=0} \tag{14}$$

instead of the $\chi_{\rm coll}(\omega)$, with a similar relation leading from the $\chi^F_{\rm osc}(\omega)$ to the oscillator response $\chi_{\rm osc}(\omega)$ for q-motion. The latter is then specified by the transport coefficients $\gamma = k^{-2}\gamma^F$, $M = k^{-2}M^F$ and $C = k^{-2}C^F$.

Whether or not such an ideal situation is actually met depends largely on the value of the coupling constant k. In fair approximation one may say it to be given whenever in (10) the static stiffness $C(0)$ is small compared to the static response $\chi(0)$. In such a case the strength of all the solutions of the secular equation $1/k + \chi(\omega) = 0$ will concentrate in the low frequency domain. Therefore it is important to realize that the static energy may depend strongly on temperature. For nuclear physics, for instance, the $C(0)$ drops dramatically above $k_BT = 2$ MeV where the influence of shell structure has diminished (see e.g.[25]).

In the more general case the strength distribution of the collective modes, which is determined by the imaginary part $\chi''_{qq}(\omega)$ of the qq-response function, will spread over several (or even many) modes. In this case the equation of motion for $q(t)$, which may be obtained from

$$\left(\chi_{qq}(\omega)\right)^{-1}\, q(\omega) = -q_{\rm ext}(\omega) \tag{15}$$

after a Fourier transform back to time, will contain terms being non-local in time which cannot be expressed simply by a sum of derivatives of $q(t)$ up to second order. If one still wants to stick to differential form one needs to apply a further approximation. For instance, one may simply expand the $\left(\chi_{qq}(\omega)\right)^{-1}$ in (15) to second order in ω [22]. Another possibility is found in "reducing" the $\chi_{qq}(\omega)$ to the $\chi_{\rm osc}(\omega)$. By this we mean to replace the former by the latter in a certain range of frequencies. In practice this may be done by fitting the imaginary part of $\chi_{\rm osc}(\omega)$ to that peak in $\chi''_{qq}(\omega)$ the corresponding mode of which one wants to treat. Notice please that both of these approximations require that only frequencies are relevant which lie in some limited regime. In this sense the second one may be considered superior to the former. In the past, various computations of transport coefficients have been performed which lead to values being in fairly good agreement with experimental experience, see [23], [22].

2.3 Unstable modes

The oscillator response is analytic in the stiffness C. As we will see below, the latter becomes negative whenever the static stiffness $C(0)$ becomes negative, which happens in the region of potential barriers where the system is unstable, in the sense that one of the two fundamental solutions for average motion begins to grow exponentially. Such a situation can still be handled within the locally harmonic approximation as long as the forces do not change too rapidly with the coordinate. Recall please that at some given Q_0 the harmonic solution is meant to portray the true one only within a limited time interval δt anyhow. This growth of the time dependent solution reflects itself in the feature that for negative C one of the poles of the collective response moves into the upper part of the frequency plane. (Notice please that the instability we have in mind still leaves both inertia as well as friction positive). This does not cause any problems when dealing with the functional form of the oscillator response as given by (12), but it may well be so for more general expressions. For instance, one may want to write the response function in terms of integral representations, like

$$\chi_{\mu\nu}(\omega) = \int_{\mathcal{C}} \frac{d\Omega}{\pi} \frac{\chi''_{\mu\nu}(\Omega)}{\Omega - \omega} \qquad \text{for } \mathrm{Im}\,\omega > 0\,. \tag{16}$$

In this case some caution is required in defining the contour $\mathcal{C}$. For stable systems it is taken along the real axes with the poles lying below. This choice is required by causality. If the same principle is still to be valid for the case of an instability the contour $\mathcal{C}$ must still be chosen to be above the one singular pole mentioned before. Actually, besides this "retarded" function it may become desirable to have an "advanced" response function as well, for which the contour then has to be modified to lie below the poles which correspond to motion backward in time. More details of these formal techniques are described in Appendix A.

2.4 Implications from sum rules

The integral representation (16) may serve as a starting point for deriving and exploiting sum rules, even in the case of instabilities. Generalizing the common definition to

$$S^{(n)}_{\mu\nu} = \int_{\mathcal{C}} \frac{d\omega}{\pi} \omega^n \chi''_{\mu\nu}(\omega)\,, \tag{17}$$

the same relations are recovered for the unstable case as those known for the stable one, if one only observes the appropriate choice of the contour. For example, for $n = -1$ the value of the integral in (17) gives the static response, $S^{(-1)}_{\mu\nu} = \chi_{\mu\nu}(\omega = 0)$, while for $n = 1$ one may employ the usual arguments to obtain

$$S^{(1)}_{\mu\nu} = \int_{\mathcal{C}} \frac{d\Omega}{\pi} \Omega \chi''_{\mu\nu}(\Omega) = \lim_{\omega\to\infty} \omega \int_{\mathcal{C}} \frac{d\Omega}{\pi} \frac{\chi''_{\mu\nu}(\Omega)}{1 - \frac{\Omega - i\varepsilon}{\omega}} = -\lim_{\omega\to\infty} \omega^2 \chi_{\mu\nu}(\omega)\,. \tag{18}$$

One way of getting the equality in the middle is to involve the geometrical series for the $1/(1 - (\Omega - i\varepsilon)/\omega)$, which is possible whenever the $S^{(n)}_{\mu\nu}$ remain finite for $n > 0$. The latter restriction is not really necessary. One may simply replace the Ω in the first integral by

$\Omega = \omega(1+\Omega/\omega) = [1-(\Omega/\omega)-(\Omega/\omega)^2/(1+\Omega/\omega)]^{-1}$ and observe that for $\omega \to \infty$ the last term in the brackets gets less and less important. Then one only needs to have the $S^{(0)}_{\mu\nu}$ vanish, which in our case is no problem as later on we are going to apply (18) only for the diagonal case. Please observe that for the oscillator response (12) the validity of the expression on the very right follows directly from inspection.

The sum rules for $n = \mp 1$ are intimately related to two of the three transport coefficients. This can be inferred from the values these two sums take on for the oscillator response, namely

$$S^{(-1)}_{\rm osc} = \frac{1}{C} \qquad S^{(1)}_{\rm osc} = \frac{1}{M} \qquad \text{with} \quad S^{(0)}_{\rm osc} = 0\,. \tag{19}$$

For later purpose we may note here that these results remain unchanged when the oscillator is modified by introducing a frequency dependent friction $\gamma = \gamma(\omega)$.

As the oscillator response is derived from the original, microscopic expression given by (3) together with (14), the sum rules may be used to derive inequalities for the transport coefficients. How these inequalities come about may best be seen writing the full response function in terms of a pole expansion like

$$\chi_{qq}(\omega) = -\sum_\alpha \frac{1}{2M_\alpha \mathcal{E}_\alpha}\left(\frac{1}{\omega-\omega^+_\alpha} - \frac{1}{\omega-\omega^-_\alpha}\right) \tag{20}$$

with $\omega^\pm_\alpha = \pm\mathcal{E}_\alpha - i\Gamma_\alpha/2$. Then one may deduce results like those given in (19) for each term of the sum over α. It is then evident that the value of the $S^{(\pm 1)}$ for each term cannot be larger than the corresponding value of the total sum.

Let us look at the inertia first. The form (3) implies $\lim_{\omega\to\infty}\omega^2(\chi_{\rm coll}(\omega)-\chi(\omega)) = 0$. Therefore we get

$$k^{-2}\,S^{(1)}_{qq} = \int_{-\infty}^{+\infty}\frac{d\Omega}{\pi}\,\chi''_{\rm coll}(\Omega)\,\Omega = \int_{-\infty}^{+\infty}\frac{d\Omega}{\pi}\,\chi''(\Omega)\,\Omega = \frac{i}{\hbar}\langle[\hat{\dot{F}},\hat{F}]\rangle \tag{21}$$

and consequently

$$\frac{1}{M} \le S^{(1)}_{qq} = \frac{ik^2}{\hbar}\langle[\hat{\dot{F}},\hat{F}]\rangle \equiv \frac{1}{m_0} \tag{22}$$

which means that the inertia for the one mode we have chosen to pick cannot be smaller than the m_0 given by the microscopic value of the energy weighted sum. In nuclear cases this m_0 can be seen to correspond to the inertia one would get in the liquid drop model for irrotational flow (see e.g. [20]).

Next let us look at the stiffness. Here the situation is slightly different as the mode we like to look at explicitly may become unstable. However, assuming that all the other ones remain stable one may simply repeat the arguments from before such that for $S^{(-1)} \equiv \chi_{qq}(0)$ one gets

$$\frac{1}{C} \le \chi_{qq}(0) \;= k\frac{\chi(0)}{\frac{1}{k}+\chi(0)} = \frac{1}{C(0)}\,\frac{\chi(0)}{\chi(0)+C(0)}. \tag{23}$$

These expressions for $\chi_{qq}(0)$ are obtained after observing (3), (14) and (10). The last equation shows the $\chi_{qq}(0)$ to have the same sign as the static response $C(0)$, from which observation

it follows that C will become negative as soon as $C(0)$ is negative. In these arguments we have assumed the static *intrinsic* response $\chi(0)$ to be positive, as there is no reason to expect the intrinsic system to be unstable. As mentioned before, we want to stick to the case where this value is larger than the absolute value of the static stiffness. The inequality allows one to prove that effective stiffness cannot be smaller than the static one:

$$C \geq C(0) \tag{24}$$

For stable modes this is immediately clear, for unstable ones it is useful to make a detour and introduce the absolute values $C = -\mid C \mid$ and $C(0) = -\mid C(0) \mid$, in which way one gets from (23)

$$\frac{1}{\mid C \mid} \geq \frac{1}{\mid C(0) \mid} \frac{1}{1 - \mid C(0) \mid / \chi(0)} \geq \frac{1}{\mid C(0) \mid} \, . \tag{25}$$

The inequality (24) expresses in clear fashion that in general the effective stiffness C will be different from the static one, $C(0)$. The reason for this difference is found in *dynamical* effects contributing to the effective potential. It is interesting to note that at an instability these effects actually *lower the absolute value of the stiffness*, opposite to the case in stable modes. In this sense the dynamics weakens the instability by *de*-creasing the conservative force.

2.5 Inferences for the high temperature limit

Two body Hamiltonians of the type (2) are frequently used in nuclear physics. Commonly, however, the notion of the coupling constant k is just taken in literal sense, namely to be a given parameter which does neither change with deformation Q nor with temperature T (see e.g. the review [29]). This is an essential difference to the situation described above for which k does depend both on Q and T, as given by (10). To see the implications of the variation with Q would require more extensive studies, which are to be deferred to the future. In particular, it would be necessary to extend the present treatment to the multi-dimensional case, as given for genuine quadrupole vibrations, for instance. Such a procedure is possible, in principle (see e.g. [12]), but it involves efforts much beyond the present study. For the T dependence, on the other hand it is quite easy to see important consequences, even at a qualitative level by simply looking at the limit one would get for the collective mode when increasing the nuclear excitation.

In the last decade or so, rather fancy procedures have been adapted from field theoretical methods to study collective dynamics at finite T. Some of them exploit the concept of small amplitude vibrations about some given thermal state of the system, like RPA at finite temperature (see e.g.[29]) or the variants of the "Static Path Approximation" such as the P(erturbed)SPA of [30] or the C(orrelated)SPA of [31]. Also there separable two body interactions similar to the one given in (2) are exploited (with the k being some given constant, it is understood). One of the striking results is that with increasing T the vibrational modes turn into the unperturbed excitations of the nucleonic degrees of freedom, even for those which at $T = 0$ would show the typical collective behavior. In our opinion, this feature contradicts basic concepts of Niels Bohr's model of a compound nucleus. The latter is dominated by

the effects of strong (incoherent) two body correlations, or, to use a word which draws more on analogies with transport theory, by the effects of two body collisions. There can be little doubt that the latter will become the more important the larger the thermal excitation (c.f. the Ansatz for the nucleon's self-energy suggested by (11)). One may then legimately ask, why it should be possible for the *independent* particle motion configurations to dominate the dynamics at large T?

At this stage it may be very worth while to recall the essence of the Strutinsky renormalization of the total static energy. For small excitations the variation of the latter is completely determined by shell effects. However, what remains when they are gone is the liquid drop energy. Consequently, the vibrations of the nucleus should behave more like those of a "drop" of nuclear matter showing largely "macroscopic" behavior, rather than that of independent particle motion. This is indeed what one gets from the theory described in the present paper (see e.g.[25] or [12], with further references given therein). As mentioned previously, with decreasing shell effects the coupling constant drops to its macroscopic limit. Consequently, the modes get very soft. Even more important is a strong concentration of strength in just *one broad collective mode*. The large width associated with this has to be understood as clear signature of strong damping, the latter feature being inherently related to the strong correlations mentioned previously. Unfortunately, the strength distribution of isoscalar modes has not yet been measured for finite temperature. Such a measurement would be an ideal test of the transition to the macroscopic limit [25], [12]. However, this transition reflects itself in transport coefficients for slow large scale collective motion like fission, in particular in their temperature dependence. Within the theory described above one finds that damping increases with T, which is in at least qualitative agreement with experimental findings, see [23] and [22]. It should be noted that the relevant quantity is not the friction coefficient itself, but combinations with those of stiffness and inertia, depending on which quantities one looks at. Whereas the T-dependence of the stiffness is well known and can be deduced from calculations of the static energy, this is less clear for the inertia. It has been shown first in [32] that one of the consequences of the T-dependent coupling constant k of (10) is a behavior of $M(T)$ as one would expect for a transition to the macroscopic limit: At small excitations the M shows the typical features of the cranking model, but above the point where shell effects have disappeared M approaches values similar to those of irrotational flow.

3 Extension to dynamical fluctuations

In the more general sense our treatment so far has not gone beyond a mean field approximation. It is true, however, that the dynamics in the basic quantities $\langle \hat{F} \rangle_t$ or $q(t)$ may be damped. Microscopically this damping implies that we need at least to consider effects which are not contained in a pure Hartree (or Hartree-Fock) approximation. However, it still suffices to stick to a description in terms of self-energies in the single particle degrees of freedom [12] and the $q(t)$ still simply is a c-number. Evidently the latter restriction has to be given up whenever one is interested to describe processes where fluctuations in the collective degrees

of freedom become relevant. Take the example mentioned before, the decay out of a potential minimum. One knows from the pioneering work of Kramers [6] how in the realm of classical physics the dynamics of fluctuations across the barrier can be treated and how they influence the decay rate. In [33] it was shown how the quantal extension of this decay rate can be obtained within a description based on transport equations. Some of the ideas behind this derivation were borrowed from the method developed in [18]. Unfortunately, also this method was again based on functional integrals for which reason it can be applied only to the schematic cases mentioned in the introduction. In this section we thus would like to proceed describing the basic steps needed for a formulation in terms of transport equations, with an elaborate discussion to come in the last two sections of the paper about the essential ingrediences of this transport equation. By those we mean these quantities which are intimately associated to fluctuations, namely the coefficients which parameterize the diffusion process in collective phase space.

3.1 Quantization of the collective variables

As the first step we need to render the collective degree of freedom to become a fluctuating variable. Often people are tempted to do this simply by adding to the Hamiltonian (8) a kinetic energy term like $\hat{\Pi}^2/(2m)$, with some unknown mass parameter m to represent the collective inertia and $\hat{\Pi}$ being the momentum conjugate to the coordinate, which then is to be considered an operator $\hat{Q}$. It is not difficult to convince oneself that in this way self-consistency would badly be lost; for a detailed discussion see [12]. This feature cannot be cured by playing with the potential part, which means to say by adding some function of $Q - Q_0$. Rather one needs to introduce a momentum dependent coupling.

Starting from the effective Hamiltonian (2) in the original particle space, this method allows one to deduce the following Hamiltonian for the total system (see [11]):

$$\mathcal{H} = \hat{H}(\hat{x}_i, \hat{p}_i, Q_0) + k\hat{\Pi}\dot{\hat{F}} - \frac{\beta}{k}(\hat{Q} - Q_0)\hat{F} + \frac{\hat{\Pi}^2}{2m_0} + \frac{(2\beta + k)}{2k^2}(\hat{Q} - Q_0)^2 \tag{26}$$

Comparing with (1) one easily identifies the parts for bare intrinsic and collective motion, as well as the coupling between both, which here consists of the two terms being linear in Π and $Q - Q_0$. In (26) the $\dot{\hat{F}} = i\,[\hat{H}(\hat{x}_i, \hat{p}_i, Q_0), \hat{F}]$, the $\hat{\Pi}$ stands for the canonical momentum and m_0 is the inertia which by (22) was introduced to represent the energy weighted sum, and which serves here to define the unperturbed collective kinetic energy. The parameter β has to be specified only in connection to the collective momentum, a point to which we will come to below. This β drops out of any equation of motion which only involves the collective coordinate Q. This feature is very similar to the properties we found before for average dynamics (as expressed in $\langle\hat{F}\rangle$ or in q) which could be traced back to the response function (3). It should be no surprise that the same function appears again when the dynamics for average motion in $q(t)$ is re-derived from Ehrenfest's equations to (26). We may note in passing that in the original version of the Bohm-Pines procedure, as it had been developed for the electron gas in [10], no such additional parameter β was needed. The difference to our

case lies in the fact that we want to apply the method to an attractive two body interaction in contrast to the repulsive one of the electron gas (c.f.[11]).

The description in terms of the Hamiltonian (26) is not yet complete. As it stands the $\mathcal{H}$ would have too many degrees of freedom and in this sense could not be equivalent to the original two body Hamiltonian $\hat{H}^{(2)}$ of (2). Indeed, the Bohm-Pines procedure necessarily involves a subsidiary condition which for the present case reads

$$k\hat{F} = \hat{Q} - Q_0 \tag{27}$$

It is nothing else but the "operator version" of the self-consistency condition (7). This property and the very fact that it is inherently incorporated into the form (26) of the Hamiltonian $\mathcal{H}$ makes it very plausible that the description of collective motion on average is the same as before. The new feature is seen in the fact that now we are in a position to treat fluctuations in the $\hat{q}$ in the way similar to what the Hamiltonian $\hat{H}^{(2)}$ of (2) allows one to do for the microscopic quantity $\hat{F}$. This feature goes along with the fact that in (26) no two body interaction appears anymore. Rather, its effects are hidden in the terms involving collective coordinate and momentum.

With the Hamiltonian (26) one may proceed to derive effective equations of motion for the propagation in collective phase space. In this spirit the Nakajima-Zwanzig projection technique has been applied in [7] to get the transport equation for the Wigner function of the collective density. However, to account for self-consistency not only on the level of average dynamics, or on that of the mean field, a non-perturbative method had to be developed for treating the integral kernel. Again this was possible within the locally harmonic approximation for which it suffices to know the propagators for the consecutive time steps δt with $\delta t \ll \tau_{\rm coll}$. As for $\delta t \to 0$ this propagator starts at a definite point in phase space, it was argued that a Gaussian approximation would do. Thus one only needs to specify the time evolution of the first and second moments. For this non-perturbative Nakajima-Zwanzig equation it was possible to prove that it is in accord with the (quantal) fluctuation dissipation theorem (FDT) [7], which in full glory requires to have non-Markovian equations of motion. This feature makes it possible to take advantage of the FDT for establishing the approximate equations of motion, which for the first and second moments may be taken to be of differential form.

3.2 Harmonic approximation for first and second moments

For average dynamics we have seen the differential equation of motion to come up through the reduction of the "full" response function (3) (or the one of (14)) to that of the oscillator given in (12). Evidently, one would like to have the equations of motion for the second moments to be of similar type. Clearly, in addition to the coordinate they will involve the collective velocity or the corresponding momentum as well. Let us first introduce the latter on the level of first moments, i.e. for $q_c(t) \equiv \langle \hat{q} \rangle_t$ and $p_c(t) \equiv \langle \hat{p} \rangle_t$. It is clear that for the harmonic case

we are looking at, one expects the following set:

$$M\frac{d}{dt}q_c(t) = p_c(t) \qquad \frac{d}{dt}p_c(t) = -\gamma\frac{d}{dt}q_c(t) - Cq_c(t)\,, \tag{28}$$

As the first equation tells one, the momentum appearing here is the kinetic one, called p henceforth. It is here where one may benefit from having the parameter β appearing in (26). As shown in [11] and [7], the choice $\beta+k = k^2C$ allows one to replace the canonical momentum Π by the kinetic one not only for average motion but also for the fluctuations around it. As demonstrated in [7] these fluctuations satisfy the following linear set of equations

$$\frac{d}{dt}\Sigma_{qq}(t) - \frac{2}{M}\Sigma_{qp}(t) = 0 \tag{29}$$

$$\frac{d}{dt}\Sigma_{qp}(t) - \frac{1}{M}\Sigma_{pp}(t) + C\Sigma_{qq}(t) + \frac{\gamma}{M}\Sigma_{qp}(t) = D_{qp} \tag{30}$$

$$\frac{d}{dt}\Sigma_{pp}(t) + 2C\Sigma_{qp}(t) + \frac{2\gamma}{M}\Sigma_{pp}(t) = 2D_{pp} \tag{31}$$

The second moments are defined as $\Sigma_{qq}(t) = \langle\hat{q}^2\rangle_t - q_c^2(t)$, and similarly for the combinations $\{q,p\}$ and $\{p,p\}$. It is seen that the structure of the homogeneous parts follow from that of (28), for which reason the $q_c^2(t)$ etc. satisfy the set (29) to (31) with the inhomogeneities $D_{qp},\ D_{pp}$ put equal to zero. For any finite value of these diffusion coefficients D_{qp} and D_{pp} the fluctuations will become finite in the course of time. This will be so even for zero initial values, as it is the case when the solutions are to represent the second moments of the propagators (see above and below). So far the diffusion coefficients have not been specified. It is here where we may benefit from the FDT. As is easily verified, these diffusion coefficients can be expressed by the stationary solutions of (29) to (31). Let us first take the conventional case of a positive C for which these stationary solutions are those of equilibrium such that we may write:

$$D_{pp} = \frac{\gamma}{M}\Sigma_{pp}^{\rm eq} \qquad D_{qp} = C\Sigma_{qq}^{\rm eq} - \frac{1}{M}\Sigma_{pp}^{\rm eq} \tag{32}$$

In the next chapter we will exploit the (quantal) FDT to evaluate these expressions. Afterwards we will turn to the case of an instability with $C < 0$ which will be handled by analytic continuation.

Often one encounters cases of strongly over-damped motion. It is not difficult to convince one-selves (see [12] and c.f.[6]) that in this case the set of equations reduces to (29) to (31)

$$\frac{d}{dt}\Sigma_{qq}(t) + 2\frac{C}{\gamma}\Sigma_{qq}(t) = 2D_{qq}^{\rm ovd} \tag{33}$$

with the diffusion coefficient $D_{qq}^{\rm ovd} = C\Sigma_{qq}^{\rm eq}/\gamma$

It may be helpful to the reader to add some further comments on the seemingly Markovian nature of our basic equations of motion. There can be no doubt that approximations of this kind are necessary in one way or other. However, for average dynamics this step to differential form does involve less stringent conditions than one would expect on usual grounds. This

feature is intimately related to the construction of the oscillator response or the definition of the transport coefficients $M,\ \gamma$ and C. Look once more at (3) and suppose that the microscopic response $\chi(\omega)$ can be represented by a Lorentzian, or its dissipative part, rather, which often may portray a realistic situation quite well. For such a case the form (12) follows without any additional approximation. On the other hand, it is almost evident that the set of equations (29) to (31) for the second moments can hardly be correct for all times t and in particular not for very small t. This set supposes that we use it for large times, a feature already suggested by our way of calculating the diffusion coefficients: They are chosen in such a way as to warrant that the set (29) to (31) describes correctly the relaxation to the proper equilibrium.

3.3 Treatment of large scale motion

The information contained in (28) to (31) may now be used to construct the time evolution in global sense. Two possibilities come to one's mind. First of all and as indicated before, one may take the first and second moments to define a Gaussian. The latter may be constructed such as to represent motion within the time lapse $\delta t = t_2 - t_1$ and which at $t = t_1$ starts from some point $Q_1,\ P_1$ in phase space. For a sufficiently short interval δt the widths $\Sigma_{\mu\nu}(t)$ may be assumed to remain small such that this motion remains restricted to a narrow region in phase space, thus justifying the linearization procedure we started off. As this propagation can be performed for any point $Q_1,\ P_1$, one may in the end sum up all possibilities needed to construct the time evolution of any initial distribution and even over time intervals of macroscopically large size. That this "propagator method" may be used even to describe such complex problems as the decay out of a potential minimum has first been demonstrated in [34].

Numerically this method turns out to be time consuming as the "summation over all possibilities" requires integration over the phase space not only for the first step but for each following intermediate step as well. It so turns out that it is simpler to translate it to the picture of a Langevin force. There one follows individual trajectories and constructs the final distribution by repeating this latter procedure for a suitably large manifold of points representing the initial distribution (in global sense). These trajectories are constructed in such a way that for the elementary time step $\delta t = t_2 - t_1$ one first moves along the average trajectory, say by solving the set (28), to find the point representing the actual position at time t_2 by Monte Carlo techniques. This sampling is to be performed by taking into account the size the fluctuation attains at $t = t_2$ according to the fluctuating force, which in turn may be determined from the information contained in the diffusion coefficient.

4 Diffusion coefficients for stable modes

To evaluate the diffusion coefficients from (32) we need to calculate the values the fluctuations would take on if the (collective) system were in equilibrium locally. The fluctuation dissipation

theorem implies

$$\Sigma^{\rm eq}_{\nu\mu} = \hbar \int \frac{d\omega}{2\pi} \coth\left(\frac{\hbar\omega}{2T}\right) \chi''_{\nu\mu}(\omega)\,. \tag{34}$$

Here the indices ν, μ are supposed to represent q and p. Exploiting the relations $\chi''_{qp}(\omega) = iM\omega\chi''_{qq}(\omega)$ and $\chi''_{pp}(\omega) = (M\omega)^2\chi''_{qq}(\omega)$, all fluctuations can be expressed by the one response function χ_{qq}. The different behavior of q and p under time reversal causes the cross term to vanish, i.e. $\Sigma^{\rm eq}_{qp} = 0$. Formally this is reflected by χ''_{qp} being even in ω. It is for this reason, that no diffusion coefficient appears in (29).

Actually, the values given by (34) are not yet suitable for our purpose. It was mentioned before that the equations (29) to (31) should be consistent with those for average motion given in (28). As the latter are derived from the oscillator response we are forced to take the latter also when evaluating the fluctuations from an expression like (34). In other words, the diffusion coefficients ought to be calculated from relations like (32) but where the $\Sigma^{\rm eq}_{\mu\nu}$ are replaced by those for the oscillator $\Sigma^{\rm osc}_{\mu\nu}$,

$$D_{pp} = \frac{\gamma}{M}\Sigma^{\rm osc}_{pp} \qquad \text{and} \qquad D_{qp} = C\Sigma^{\rm osc}_{qq} - \frac{1}{M}\Sigma^{\rm osc}_{pp}\,, \tag{35}$$

and the equilibrium fluctuations are finally to be calculated from

$$\Sigma^{\rm osc}_{qq} = \hbar \int \frac{d\omega}{2\pi} \coth\left(\frac{\hbar\omega}{2T}\right) \chi''_{\rm osc}(\omega) \tag{36}$$

and

$$\Sigma^{\rm osc}_{pp} = M^2\hbar \int \frac{d\omega}{2\pi} \coth\left(\frac{\hbar\omega}{2T}\right) \omega^2\, \chi''_{\rm osc}(\omega)\,. \tag{37}$$

In doing so we keep the $\Sigma^{\rm eq}_{qp} = 0$ *untouched*, as it results from a fundamental symmetry.

4.1 Limiting cases

Before turning to the general case let us look at the limits of high temperature and of small damping. The former is established if the argument of the hyperbolic cotangent is small, i.e. $\hbar\omega/(2T) << 1$, for all frequencies which contribute to the integrals. Quite generally, one finds: $\Sigma^{\rm eq}_{\nu\mu} = T\chi_{\nu\mu}(\omega = 0)$ which for the oscillator leads to the classical equipartition theorem:

$$\frac{\langle\, \hat{P}^2 \,\rangle_{eq}}{2M} = \frac{T}{2} = \frac{C\langle\, \hat{q}^2 \,\rangle_{eq}}{2}. \tag{38}$$

As a consequence, for the diffusion coefficient one obtains the classic Einstein relation

$$D_{pp} = \gamma T \qquad \text{with} \qquad D_{qp} = 0 \tag{39}$$

Notice that for this result no assumption was necessary about the strength of the friction coefficient, besides the fact that γ will influence the range of frequencies which must be considered small compared to T.

In the limit of zero damping one finds a similar result, only that the temperature T has to be replaced by an effective one, namely

$$T^*(\varpi) = \frac{\hbar\varpi}{2} \coth\left(\frac{\hbar\varpi}{2T}\right) \tag{40}$$

with $\varpi^2 = |C|/M$. This is easily verified letting the friction γ in the oscillator response (12) go to zero. Then the dissipative part of the response function can be written as

$$\lim_{\gamma\to 0} \chi''_{\rm osc}(\omega) = \frac{\pi}{2M\varpi} \left(\delta(\omega-\varpi) - \delta(\omega+\varpi)\right) \tag{41}$$

The resulting version of the generalized Einstein relation, i.e. $D_{pp} = \gamma T^*$, has been used in [26]. It allows for a nice and simple evaluation of the correction terms to the classical relation, namely $D_{pp} \approx \gamma T(1 + (1/3)(\varpi/2T)^2$. However, as we will demonstrate below, the form $D_{pp} = \gamma T^*$ approximates the correct formula only for extremely small friction.

4.2 General case

To evaluate the integral in (34) one commonly expands the hyperbolic cotangent into the uniformly convergent series

$$\coth\left(\frac{\hbar\omega}{2T}\right) = \frac{2T}{\hbar} \sum_{n=-\infty}^{n=\infty} \frac{1}{\omega - in\Theta} \qquad\qquad \Theta = \frac{2\pi T}{\hbar} \tag{42}$$

and applies a general relation (see (A.5)) which allows one to evaluate the response function through its spectral density, the dissipative part; such expressions are briefly discussed in Appendix A. For the terms with positive n, the integral leads to the retarded response function calculated at the corresponding pole of the coth, namely

$$\int_{\mathcal{C}} \frac{d\omega}{\pi} \frac{\chi''_{\nu\mu}(\omega)}{\omega - i|n|\Theta} = \chi^{\rm R}_{\nu\mu}(i|n|\Theta) \tag{43}$$

For negative n, one may use a relation between retarded and advanced response to find

$$\int_{\mathcal{C}} \frac{d\omega}{\pi} \frac{\chi''_{\nu\mu}(\omega)}{\omega + i|n|\Theta} = \left(\chi^{\rm R}_{\mu\nu}(i|n|\Theta)\right)^* \tag{44}$$

Notice please that in the classical limit it is only the term with $n = 0$ which survives and which leads to $T\chi_{\nu\mu}(\omega = 0)$. The quantum corrections are caused by those contributions to (42) having a finite n.

A straightforward calculation then shows the diagonal case elements $\Sigma^{\rm eq}_{\mu\mu}$ to be given by

$$\Sigma^{\rm eq}_{\mu\mu} = T\left(\chi_{\mu\mu}(\omega = 0) + 2\sum_{n=1}^{\infty} \chi_{\mu\mu}(in\Theta)\right) \tag{45}$$

In this expression we have used the fact that the response function $\chi_{\mu\mu}$ is real along the imaginary axis.

To evaluate the diffusion coefficients we need to apply (45) to the oscillator response. Unfortunately, the resulting series diverges logarithmically for the momentum fluctuations. Actually, such a behavior can better be read off from the integral (37) after recognizing that the dissipative part of (12) decreases with ω only like ω^{-3}. To cure this problem one needs to regularize the integral. In [7] the latter was simply cut off at a certain upper limit. Here we would like to apply the somewhat more elegant method of the so called Drude regularization (see e.g. [5]). It implies replacing in (12) the friction coefficient by a function of the form

$$\gamma(\omega) = \frac{\gamma}{1 - i\frac{\omega}{\varpi_D}} \,. \tag{46}$$

Properties of the resulting modified oscillator response function are discussed in Appendix B. In (46) the additional parameter ϖ_D appears, the appropriate choice of which depends on general properties of the system. In the present work we shall assume the time scale $1/\varpi_D$ to be well separated from that of collective motion and will examine how in a physically reasonable regime this parameter influences the diffusion coefficients.

For the $\Sigma^{\rm osc}_{pp}$ one finds the following expression:

$$\Sigma^{\rm osc}_{pp}(\varpi_D) = TM\left(1 + 2\sum_{n=1}^{\infty}\left[C + n\Theta\gamma(in\Theta)\right]\chi_{\rm osc}(in\Theta)\right), \tag{47}$$

A common procedure to evaluate further both (45) and (47) is to make use of the digamma function $\Psi(z) = \frac{d}{dz}\ln\Gamma(z)$. It allows one to sum up series over products of pole terms, for instance in the form (see e.g. [27, 28])

$$\sum_{n=1}^{\infty}\frac{1}{(n+y)(n+z)} = \frac{\Psi(1+y) - \Psi(1+z)}{y-z} \tag{48}$$

The oscillator response with the constant γ replaced by the one of (46) has three poles $\omega^{(i)}$ (see Appendix B). Thus one may rewrite it as a sum of three terms where each one factorizes like the left hand side of (48). After some manipulations one then ends up with

$$C\Sigma^{\rm osc}_{qq}(\varpi_D) = T\left(1 + \frac{C}{M\pi T}\sum_{j=1}^{3}\frac{\varpi_D - i\omega^{(j)}}{(\omega^{(j)} - \omega^{(j+1)})(\omega^{(j)} - \omega^{(j+2)})}\,\Psi\left(1 + i\frac{\hbar\omega^{(j)}}{2\pi T}\right)\right) \tag{49}$$

and

$$\frac{1}{M}\Sigma^{\rm osc}_{pp}(\varpi_D) = C\Sigma^{\rm osc}_{qq}(\varpi_D) + \frac{\gamma\hbar\varpi_D}{M\pi}\sum_{j=1}^{3}\frac{-i\omega^{(j)}}{(\omega^{(j)} - \omega^{(j+1)})(\omega^{(j)} - \omega^{(j+2)})}\,\Psi\left(1 + i\frac{\hbar\omega^{(j)}}{2\pi T}\right) \tag{50}$$

where the convention $\omega^{(j+3)} \equiv \omega^{(j)}$ is used. In (49) also the qq-fluctuation has been evaluated with the Drude regularization, mainly to allow for a clear comparison to the other case where this regularization is really necessary. It is clear from (46) that for large ϖ_D the result (49) will turn into the one calculated for constant friction. How rapidly this happens depends on the values of the parameters involved. This is demonstrated in Fig.1 a by numerical calculation. It is seen that large values of ϖ_D are needed for small values of temperature and

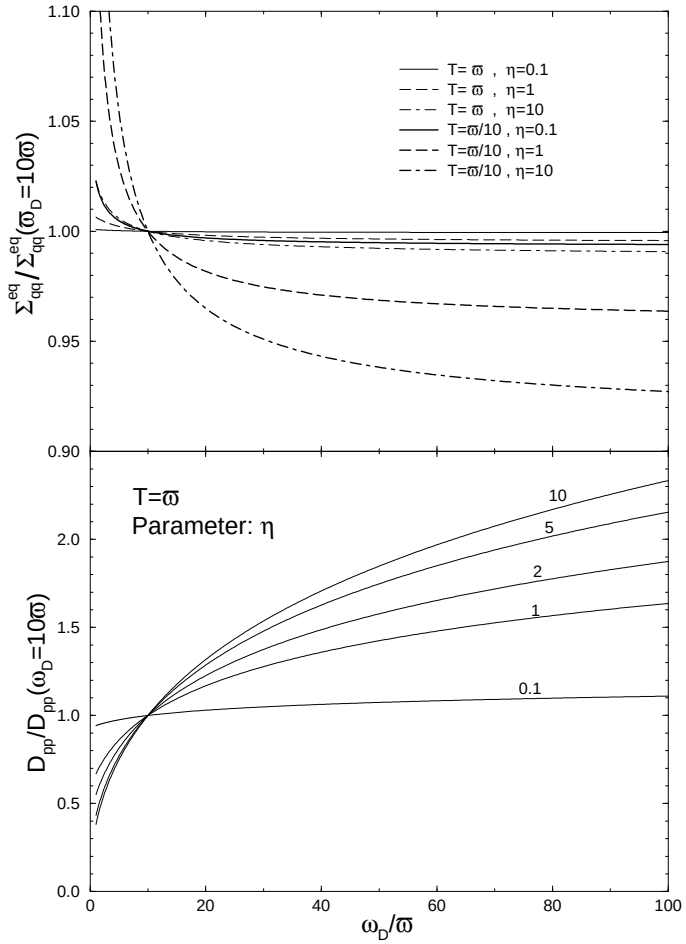

Figure 1: Equilibrium fluctuations in q (upper panel) and diagonal diffusion coefficient (lower panel) as functions of the cut off frequency for various values of damping rate η and temperature T. (The calculations are performed in units with $k_B = 1$ and $\hbar = 1$).

large damping before the asymptotic limit is really reached. It may be seen as well that even for comparatively small ϖ_D the difference to this asymptotic limit is quite small. (It should be clear from above that ϖ_D must not be chosen smaller than the typical frequencies of the original oscillator.) Here and in the following it turns out convenient to measure frequency in units of $\varpi = \sqrt{|C|/M}$ and the degree of damping by the dimension-less ratio $\eta = \gamma/(2M\varpi)$.

Different to the qq-fluctuations, those of the momentum would diverge for large ϖ_D. Therefore, one must expect them to exhibit a stronger dependence on the Drude frequency ϖ_D than seen in the $qq-$fluctuations. This is demonstrated in Fig.1.b. Indeed, for large η this dependence is quite sensible. We may notice that the diffusion coefficient increases with ϖ_D, although its classical limit is independent of ϖ_D. In this sense it can be said the quantum corrections to increase with ϖ_D, too. The standard values chosen for the figures presented here, namely $\varpi_D \approx 10\,\omega$, are probably very reasonable. Fortunately, in this region the dependence of the diffusion coefficient on ϖ_D is not very strong, the value of D_{pp} changing by 30% if ϖ_D is increased by a factor 2.

Let us turn now to the dependence of the diffusion coefficients on temperature T and on the effective damping rate η. Although the transport coefficients for average motion, M, γ and C, must be expected to vary with these parameters as well, this feature will be neglected here. All computations will be done in Drude regularization. If not stated otherwise, the value of ϖ_D will be chosen such that the ratio $\zeta = \varpi/\varpi_D$ equals 0.1. To simplify notation we want to use the same symbol as if we would use the mere oscillator, which is to say that in expressions like the ones on the left hand side of (49) and (50) the argument ϖ_D will be left out. We shall also omit the index osc at times.

Let us begin looking at the equilibrium fluctuations (see also [5]), first in the coordinate q. Rather than showing the $\Sigma^{\rm osc}_{qq}$ itself, we plot $C\Sigma^{\rm osc}_{qq}$, normalized to its value as given by the quantal ground state (Fig.2.a). Fig.2.a shows the temperature dependence for different values of η. One finds the quantum effects to disappear both with increasing T and η. The first effect

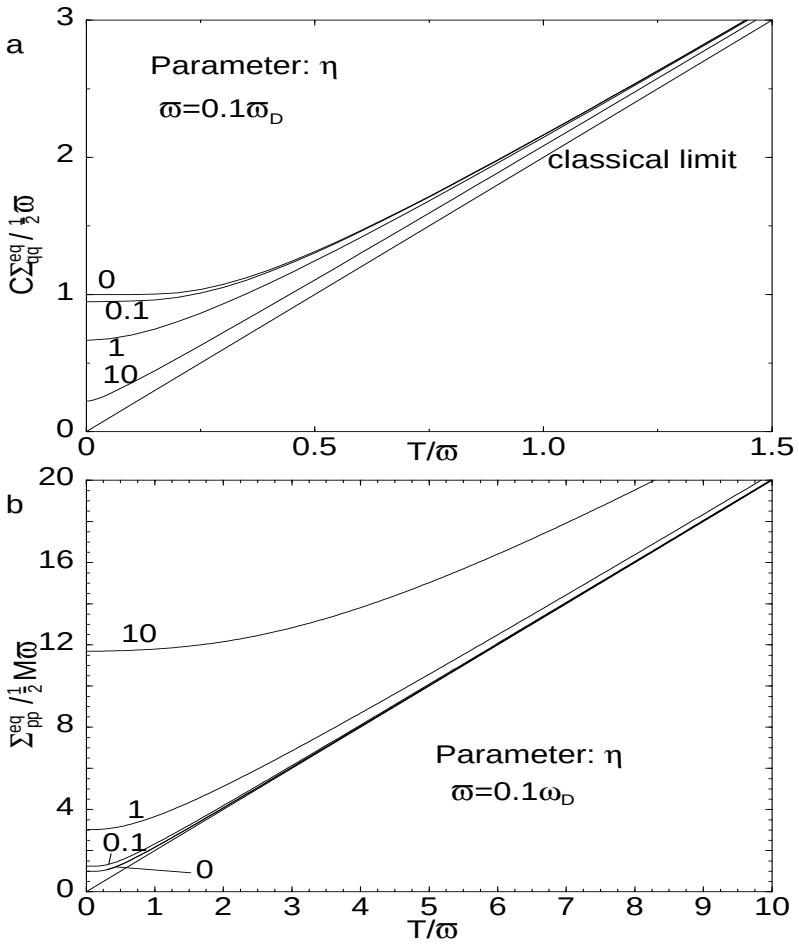

Figure 2: Equilibrium fluctuations in the coordinate (upper panel) and in the momentum (lower panel) as functions of temperature normalized to the frequency ϖ of the oscillator, for different values of the damping rate η.

is expected, although it may be somewhat of a surprise how quickly the high temperature limit is reached. The second effect causes the $\Sigma^{\rm eq}_{qq}$ to reach this limit the faster the larger the

damping. While behaving similarly with increasing T, the fluctuations in momentum differ in their dependence on η: They increase with increasing damping. This is demonstrated in Fig.2.b. Here $\Sigma_{pp}^{\rm osc}/0.5M\varpi$ (or equivalently $D_{pp}/0.5\gamma\varpi$) is plotted versus temperature for different η. This figure clearly shows how much the quantum effects are enhanced by friction. Take the regime of $T \leq \varpi$ where the change with T is quite small. For large η the fluctuations exceed several times the values they have for undamped motion.

Next we study the diffusion coefficients. They are plotted in Fig.3 by the dashed lines as function of η for different temperatures, the latter being normalized to ϖ. In Fig.3.a we

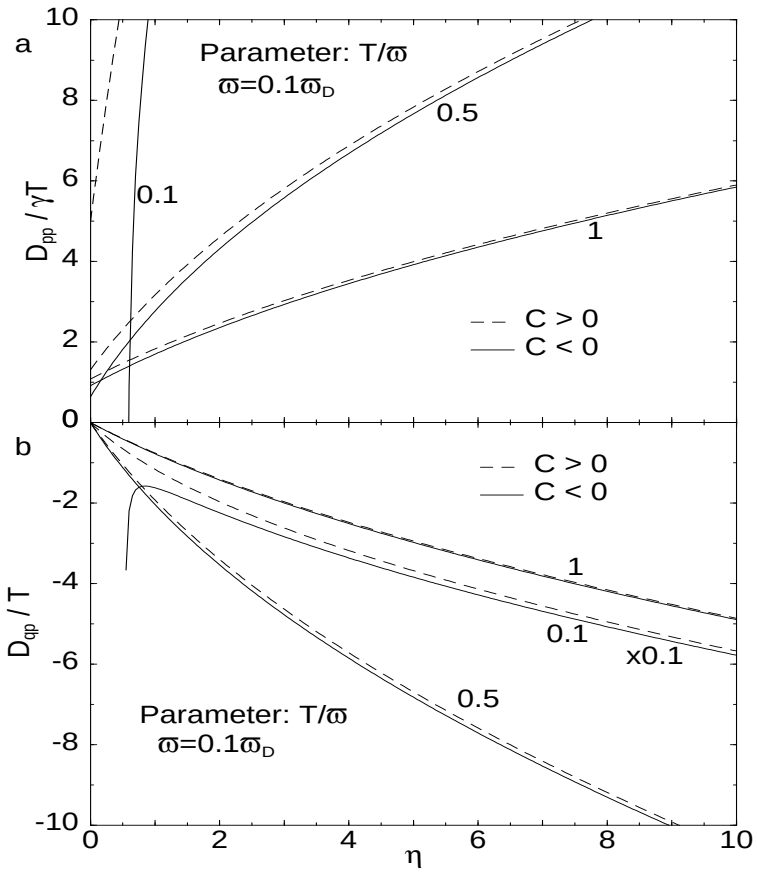

Figure 3: Diagonal (upper panel) and off diagonal (lower panel) diffusion coefficient for stable (dashed) and unstable (fully drawn) modes, as functions of the damping rate η, for three different temperatures. In the lower panel the curve for $T = 0.1\varpi$ shows $0.1D_{qp}/T$, as indicated by the symbol $\times 0.1$.

show the diagonal one, divided by its high temperature limit, $D_{pp}/\gamma T$; Fig.3.b represents the non-diagonal one, divided by temperature. Both figures demonstrate that for the diffusion coefficients quantum effects increase with damping, and that they may become quite large. Take the non-diagonal element plotted in Fig.3.b and recall its definition according to (35). It measures the difference between $C\Sigma_{qq}^{\rm osc}$ and $\frac{1}{M}\Sigma_{pp}^{\rm osc}$, which vanishes in the high temperature limit. But Fig.3.b demonstrates that for small T this difference, and thus D_{qp}, reaches values which are several times this unit. Moreover, these figures show that the "limit of zero friction"

discussed previously must be taken literally: It is obtained for such small values of friction only that it is practically never realized in nuclear physics. Look for instance at Fig.3.b: Already for $\eta > 0.5$ the D_{qp} is seen to be at least of order T even for $T \approx \varpi$, whereas in the strict limit of zero friction D_{qp} vanishes identically.

It has been mentioned that in the computations of [7] regularization of the appropriate integral had been achieved by introducing an upper limit in the integral itself, rather than to change the integrand applying the Drude regularization. The two methods are compared with each other in Fig.4. They are seen to lead to the same dependence on η but may require an optimization of the cut-off parameters, if the comparison is to become more quantitative.

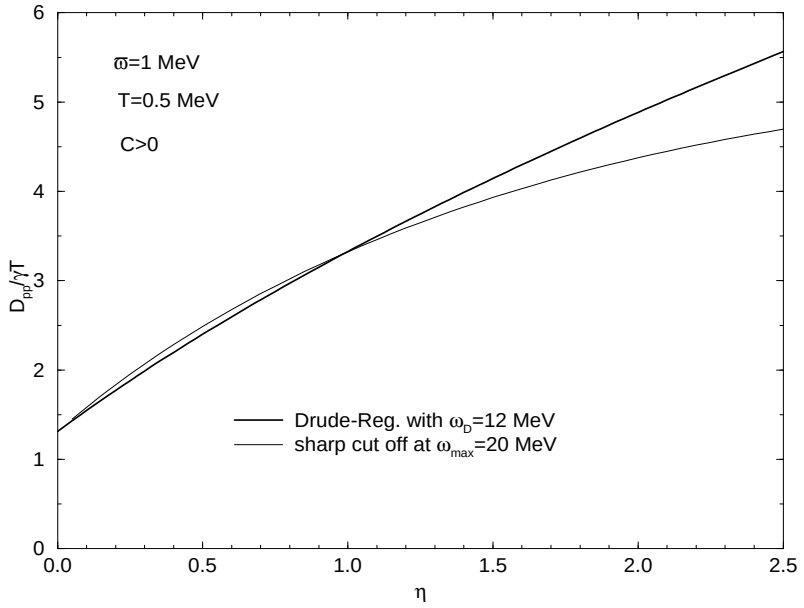

Figure 4: Comparison of two regularization schemes: Sharp cut off (thin line) and smooth cut off through Drude regularization. The values of the cut off frequencies, $\omega_{\max}$ and ω_{D} respectively, were choosen in such a way that in both cases the diffusion coefficient attains about the same value.

5 Diffusion coefficients for unstable modes

The principle which allows one to deduce diffusion coefficients from the fluctuation dissipation theorem even for unstable modes has been suggested in [9], see also [33]. In the following we like to explore this possibility in more detail with the help of formulas obtained by adapting linear response theory to instabilities. All we need to do is to generalize expressions such as (49) and (50) to the case of negative stiffness.

The basic idea is found in realizing that all the expressions derived and discussed in the previous sections are analytic expressions in the transport coefficients, and thus also in the stiffness coefficient C. This is true in particular for the general expressions for the diffusion coefficients as given by (49) and (50), together with (35). In Fig.5 we present a computation

of three typical quantities, namely $C\Sigma^{\rm eq}_{qq}$, D_{pp} and D_{qp}, all three normalized to temperature, as function of the stiffness parameter C (divided by the inertia M and relative to $(\gamma/M)^2$). The

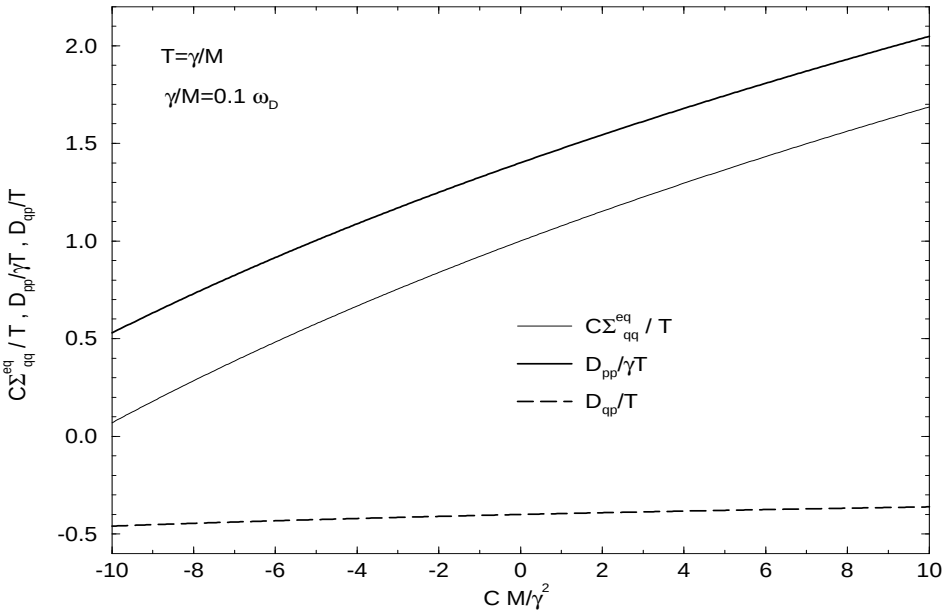

Figure 5: Diffusion coefficients (diagonal: thick fully drawn line, off diagonal: dashed line) and analytic continuation of the equilibrium fluctuations in q (thin full line) as functions of the stiffness C, for fixed values of M and γ.

result demonstrates the smoothness, or analyticity, across the point $C = 0$, which actually corresponds to the inflection point $C(0) = 0$ of the static energy. This feature is quite interesting, for several reasons. First of all one realizes that the fluctuation in the coordinate diverges when C approaches zero from above: $\Sigma^{\rm eq}_{qq} \to +\infty$ for $C \to 0^+$. Secondly, across this point this "fluctuation" gets even *negative*. Fortunately, for the equations of motion it is not this "hypothetical" *static fluctuation* which matters but the diffusion coefficients. The figure nicely demonstrates that all of *them* remain well behaved at this point implying that the same will be true for the *dynamical* fluctuations!

On the other hand, Fig.5 also demonstrates that there are limitations in applying the analytical continuation to get meaningful diffusion coefficients. It should be clear that the diagonal one ought to be positive. However, depending on the parameters involved, like the transport coefficients for average motion or temperature, the D_{pp} may become zero or even negative. This feature can be seen more clearly in Fig.6 where we plot the analytical continuations for $\Sigma^{\rm eq}_{qq}$ and $\Sigma^{\rm eq}_{pp}$ as function of temperature divided by the bare frequency, i.e. of T/ϖ. The two quantities are normalized such that in the high temperature limit they approach the same value, namely $2T/\varpi$. Actually, the factor two here is a relict of the discussion of the stable case presented in Fig.2, where the same quantities were plotted, and where this normalization was convenient at $T = 0$. Since the curves of Fig.6 just represent the analytical continuation of those in Fig.2, it is not surprising that the quantum effects behave in the same way as for stable modes when studied as functions of temperature and friction.

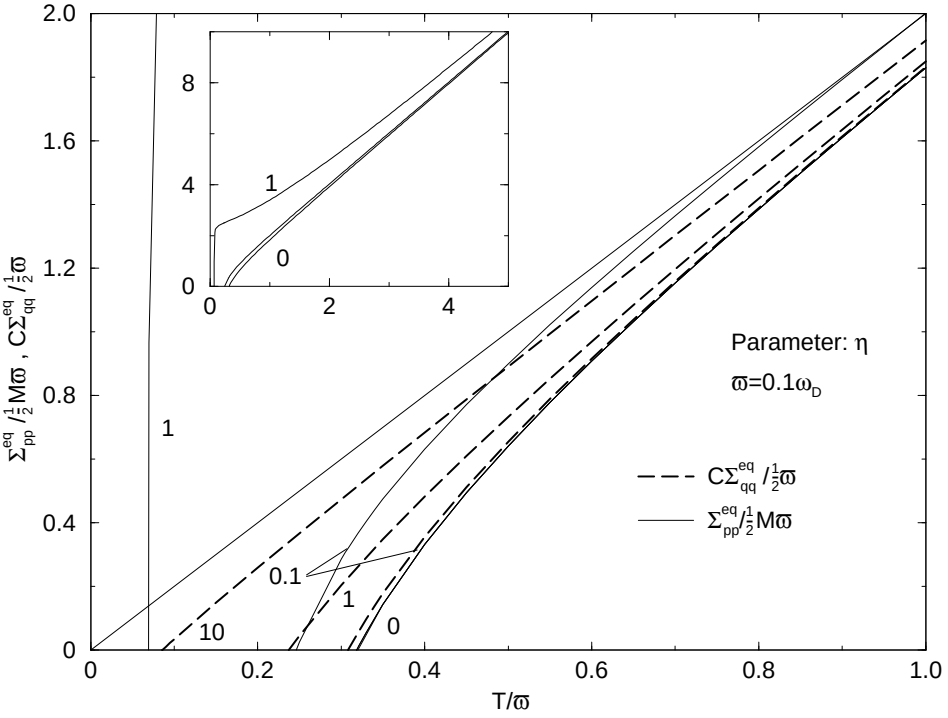

Figure 6: Analytic continuations of the (diagonal) equilibrium fluctuations to the case of negative stiffness (dashed line for the coordinate, fully drawn lines for the momentum), as functions of temperature for different values of friction. The insert shows the momentum fluctuations for a larger range of the temperature and the same values of η.

At this stage it may be worth while to refer the reader to the two easy examples discussed in the previous chapter, namely the limit of high temperature on one hand and the case of zero damping on the other one. Indeed, eq.(39) tells one that the relevant diffusion coefficient D_{pp} remains positive for all T, but from eq.(38) on sees the $\Sigma^{\rm eq}_{qq}$ to change sign at the point of inflection. On the other hand, the T^* gets negative below a critical temperature of $T_c = \hbar\varpi/\pi$. The figure Fig.6 shows such features to hold true in the general case with the following two important modifications: a) The T_c is shifted to lower values when η is increased; b) this shift is bigger for the momentum fluctuations. At larger values of η the latter even show a different behavior, in the sense that they become larger than the value given by the high temperature limit, which for larger T they approach from above.

The non-diagonal diffusion coefficient D_{qp} is plotted in Fig.7 as function of temperature, both for positive and negative stiffnesses, and in Fig.3.b by the fully drawn lines as function of friction. The values of D_{qp} for positive and negative stiffness differ from each other only for small temperatures and small friction, and practically agree with each other already for temperatures larger than about $0.5\hbar\varpi$ and friction $\eta > 2$. A similar behavior is true for the diagonal element, as may be inferred comparing fig. 3.a and Fig.6. At very small T/ϖ the D_{qp} shows an anomalous decrease with T/ϖ (see Fig.7) or with η (see Fig.3.b). This actually happens in a regime below T_c, the reason of which will be discussed on below.

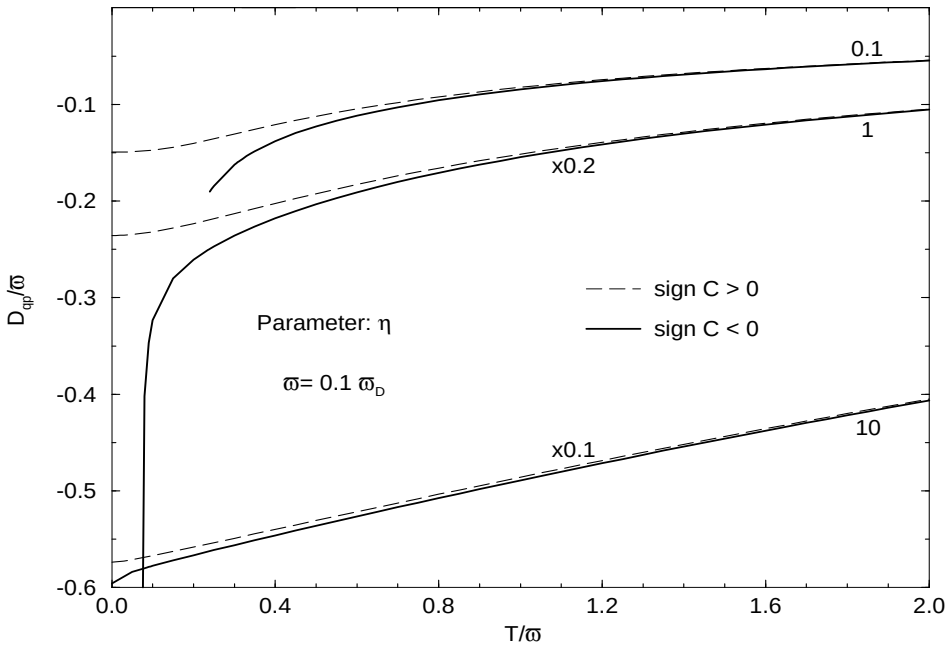

Figure 7: Off diagonal diffusion coefficient as function of temperature for three values of friction, for a stable (dashed lines) and an unstable (fully drawn lines) system. The curves for $\eta = 1, 10$ show D_{qp} multiplied by 0.2 and 0.1, respectively.

Finally, we would like to come back once more to the fluctuation dissipation theorem in its general form. We recall that it was this theorem which allowed us to determine the diffusion coefficients in terms of the response function of average motion. Furthermore, these are exactly the expressions, taken as analytical functions of the stiffness C, which we were able to generalize to unstable modes by analytical continuation from a positive stiffness to a negative one. The construction of the special contour $\mathcal{C}$ now allows us to perform these steps in a more direct fashion, provided one more constraint on the contour is considered. That is to say that at instabilities we may express the "equilibrium fluctuations" by the following integral:

$$\Sigma^{\rm eq}_{\mu\nu} = \hbar \int_{\mathcal{C}} \frac{{\rm d}\omega}{2\pi} \coth\left(\frac{\omega}{2T}\right) \chi''_{\mu\nu}(\omega) \tag{51}$$

In this integrand there appears another factor having poles in the complex plane, the coth which diverges at the Matsubara frequencies $\omega^n_{\rm M} = \pm n 2\pi T/\hbar$. As in the stable case, the contour $\mathcal{C}$ has to cross the imaginary axis in between those which lie closest to the real axis [35], namely $\pm 2\pi T/\hbar$. This condition actually puts a lower limit on the range of temperatures for which such a construction may work, namely $T > T_0 \equiv \hbar|\omega_+|/(2\pi)$, with ω_+ being the frequency of the unstable mode (see Appendix B, in particular eqs.(B.9) and (B.11) and the text below them). This follows from the constraint discussed in the context of eq.(16) according to which the contour $\mathcal{C}$ has to lie *above* the unstable pole. Actually, this T_0 coincides with the so called "cross over temperature" encountered in dissipative tunneling (see eq.(3.7) of [4]), which will be commented on in the next chapter. For illustrative purpose we may look once more at the limiting case of zero friction for which one gets $T_0 = \hbar\varpi/(2\pi)$ and thus

$2\,T_0 = T_c$. The feature of the critical temperature T_c being larger than the T_0 is generally correct.

It is interesting to note that such a minimal temperature below which motion can no longer be treated in a harmonic approximation is found also in two extensions of the SPA, called P(erturbed)SPA in [30] and C(orrelated)SPA in [31]. Both approaches are very similar to one another, in the sense that small amplitude vibrations are considered on top of or around the "static path" approximation to the functional integral — and are thus analogous in spirit to our locally harmonic approximation. Being based on a path integral formulation, it may be not very surprising that in this method the minimal temperature turns out to be identical to T_0. It must be said, however, that both in PSPA as well as in CSPA *no damping* of the modes is considered. Within our time dependent formulation the latter feature is made possible through considerations of coupling of 1p-1h-correlations to more complicated ones. In this sense the two body interaction effectively goes beyond the separable form given in (2), which just refers to the one generating collective motion. Certainly, more work will be needed to make the correspondence of these different procedures more apparent.

6 Summary and Conclusions

In this paper we have reviewed a method which allows one to describe the dynamics of damped motion in collective phase space. The main emphasize was put on the evaluation of diffusion coefficients $D_{\mu\nu}$ which govern motion of the second moments both for stable as well as for unstable modes. The latter case was handled by a suitable analytic continuation of the (quantal) fluctuation dissipation theorem. To this end some elementary properties of linear response functions had to be generalized, too.

From the numerical results it became evident that, when applied to the diffusion coefficients, this continuation looses its physical meaning below a critical temperature T_c below which even the diagonal element D_{pp} would become negative. On the other hand, for the fluctuation dissipation theorem, as well as for some basic relations of response theory, such a continuation is possible even for temperatures down to a $T_0 < T_c$. This T_0 was seen to be identical to $T_0 = \hbar|\omega_+|/(2\pi)$ where $\omega_+ = -(\omega_+)^*$ measures the position of the pole along the positive imaginary axis which belongs to the unstable mode. This T_0 is thus identical to the so called "cross over temperature" [4] one encounters in the phenomenon of "dissipative tunneling" and for undamped motion in the PSPA and the CSPA of [30] and [31], respectively.

This association to tunneling is by far not accidental. As mentioned above, the equations of motion associated to the harmonic case can be exploited for describing global motion within a locally harmonic approximation. In the end this means to describe collective dynamics by way of a transport equations like the one of Kramers, with the only difference of generalizing the classical Einstein relation to the proper quantal form. This implies to have two diffusion coefficients D_{qp} and D_{pp} instead of the single one $D_{pp} = \gamma\, T$. Applying this scheme to evaluate the rate of decay out of a potential minimum one finds [33] the formula $R = f_{\rm Q} R_{\rm K}$ known from such model cases for which an application of functional integrals becomes feasible.

Compared to this latter situation, the derivation sketched here has both an advantage as well as a disadvantage. The advantage can be found in the fact that this locally harmonic approximation can be applied to cases for which the coupling between the collective degree of freedom and the rest is too big to allow for the simplification of linearizing in the "bath variables", with the latter simply being represented by oscillators with *fixed* inertias and stiffnesses. On the other hand the description in terms of transport equations of the type mentioned is valid only for $T > T_c > T_0$. In this sense this critical temperature T_c indicates a breakdown of the locally harmonic approximation in general.

In this paper it has been emphasized that the construction of the basic equations of motion is possible in self-consistent manor. By this notion we mean that the collective degree of freedom is introduced to represent the dynamical microscopic quantity one wants to study. This is necessary for all systems which per se exist of identical particles, like it is the case for nuclei or the electron gas, to mention just two prominent examples.

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A Extension of linear response theory to unstable modes

In the presence of an unstable mode of frequency $\omega_+ = i\Gamma$ the relations between response function have to be modified as compared to the common situation of a stable system. As we are going to show in this Appendix, some relations between response function and its dissipative part can be retained by making use of deformed paths of integration in the complex frequency plane, as encountered in the text for the contour $\mathcal{C}$ of (16).

Causality requires that a physical quantity can be influenced by external fields only from their values in the past. The retarded function describing such a response must thus vanish for negative times. This may be achieved by an appropriate choice of the contour $\mathcal{C}_+$ for that integral which defines the Fourier transformation from the frequency representation back to time: For negative times, it must be possible to close this integral in the complex frequency plane without enclosing any pole of the retarded response function $\chi^{\mathrm{R}}(\omega)$. This allows one to write:

$$+\,2i\Theta(+t)\chi''(t) = \int_{\mathcal{C}_+} \frac{d\omega}{2\pi} e^{-i\omega t}\chi^{\mathrm{R}}(\omega)\,. \tag{A.1}$$

The contour $\mathcal{C}_+$ could for instance be chosen parallel to the real axis if it only lies *above* the $\omega_+ = i\Gamma$ (being the pole of χ^{R} having the largest imaginary part). In the case of the advanced

response, in (A.1) all + signs are to be replaced by − signs, with the contour $\mathcal{C}_-$ lying below all poles of the advanced function. In the following we will write both versions in combined form, using an index X to distinguish between R(etarded) and the A(dvanced). Whenever the possible signs ± will appear, the upper one will relate to the retarded, the lower one to the advanced response.

To obtain the equivalent of the well known relation between the frequency representations of response function and its dissipative part, one may start with the inversion of (A.1),

$$\chi^{\mathrm{X}}(\omega) = \pm \int dt e^{i\omega t} 2i\Theta(\pm t)\chi''(t) \qquad |\mathrm{Im}\omega| > \Gamma\,, \tag{A.2}$$

which is restricted to frequencies whose imaginary part is larger (smaller) than Γ. In a second step, one may combine (A.2) for retarded and advanced response to find an expression for the dissipative part of the response function,

$$\chi''(t) = \frac{1}{2i}\left(\int_{\mathcal{C}_+} \frac{d\omega}{2\pi} e^{-i\omega t}\chi^{\mathrm{R}}(\omega) - \int_{\mathcal{C}_-} \frac{d\omega}{2\pi} e^{-i\omega t}\chi^{\mathrm{A}}(\omega)\right). \tag{A.3}$$

Under the assumption that retarded and advanced response do not share any common pole both contours $\mathcal{C}_\pm$ may be deformed to a common one $\mathcal{C}$ without changing the value of each integral. One only has to ensure that $\mathcal{C}$ has all poles of the retarded response on one side and those of the advanced one on the other. For a stable system, $\mathcal{C}$ can be taken along the real axis and the formulas presented here turn to the ones known from the common literature.

The final step is to insert the dissipative part (A.3) into (A.2) and to exchange the order of integration for time and frequency. Defining the analytic continuation (with respect to ω) of the dissipative part of the response function by

$$\chi''(\omega) = \frac{1}{2i}(\chi^{\mathrm{R}}(\omega) - \chi^{\mathrm{A}}(\omega)) \tag{A.4}$$

one obtains the familiar form

$$\chi^{\mathrm{R}}(\omega) = \int_{\mathcal{C}} \frac{d\Omega}{\pi} \frac{\chi''(\Omega)}{\Omega - \omega} \qquad \text{for } \mathrm{Im}\,\omega > 0 \text{ and } \omega \neq i\Gamma \tag{A.5}$$

This equation is the key relation for obtaining the integral representation (51) for the fluctuation dissipation theorem from the analytic continuation of its representation (45).

B The modified oscillator of the Drude regularization

In (46) a frequency dependent friction coefficient was introduced to render some previously diverging integrals well behaved. The form chosen there, $\gamma(\omega) = \gamma(1 - i\omega/\varpi_D)^{-1}$, is commonly associated to the Drude regularization. Replacing the friction coefficient in the oscillator response (12) by this function the related dissipative part changes to

$$\chi''^{\mathrm{dru}}_{\mathrm{osc}}(\omega) = \frac{1}{2}\frac{\omega\,(\gamma(\omega) + \gamma^*(\omega))}{M(\omega^2 - \varpi^2)^2 + i\omega(\gamma(\omega) - \gamma^*(\omega))(\omega^2 - \varpi^2) + \gamma(\omega)\gamma^*(\omega)\omega^2} \tag{B.6}$$

It is apparent that with increasing ω the form on right hand side of (B.6) drops faster than the one with constant friction. Therefore, the $\chi''^{\rm dru}_{\rm osc}(\omega)$ simulates better a correct behavior of the true response function at large ω, whereas the difference to the mere oscillator response function is small in the regions of maximal strength.

The modified response function has one more pole as given by the new secular equation

$$C - i\omega\Big(\frac{C}{\varpi_D} + \gamma\Big) - M\omega^2 + i\frac{M}{\varpi_D}\omega^3 = 0 \tag{B.7}$$

Actually, its solutions depend on two parameters only, as can be seen by introducing $x = i\frac{\omega}{\varpi_D}$ and rewriting (B.7) to

$$-x^3 + x^2 - \Big(\frac{C}{M\varpi_D^2} + \frac{\gamma}{M\varpi_D}\Big)x + \frac{C}{M\varpi_D^2} = 0 \tag{B.8}$$

This equation allows for an analytic solution, but it is more convenient to just solve it numerically. It is, however, instructive to evaluate them in first order in ϖ/ϖ_D, or, less lengthy, to solve directly (B.7) perturbatively. Defining $\eta = \gamma/(2M\varpi)$ and $\zeta = \varpi/\varpi_D$, one finds for the first two solutions

$$\omega^{(1)} \approx \varpi\left(+\sqrt{\mathrm{sign}C - \eta^2} - i\eta + 2\eta\zeta\left[\tfrac{1-2\eta_C^2}{1-\eta_C^2}\sqrt{\mathrm{sign}C - \eta^2} - i2\eta\right]\right) \tag{B.9}$$

$$\omega^{(2)} \approx \varpi\left(-\sqrt{\mathrm{sign}C - \eta^2} - i\eta + 2\eta\zeta\left[-\tfrac{1-2\eta_C^2}{1-\eta_C^2}\sqrt{\mathrm{sign}C - \eta^2} - i2\eta\right]\right) \tag{B.10}$$

It is easily recognized that for $\eta\zeta \to 0$ they turn into the solutions $\omega_\pm$ for the common oscillator, with $\omega_\pm = \pm\sqrt{C/M - \gamma^2/(2M^2)} - i\gamma/(2M)$. For the third solution one finds:

$$\omega^{(3)} = -i\varpi_D(1 - 2\eta\zeta) \tag{B.11}$$

A few remarks are in order here. First of all, it is interesting to note that it is not the ratio ζ itself which matters but the combination with η. It is intuitively clear that for larger damping the Drude frequency must be chosen larger. Secondly, we see that for a large ϖ_D, at least, the third pole lies on the negative imaginary axis.

Let us finally just write down an expression for the full response function which serves as starting point for expressing the fluctuations in terms of the $\Psi-$function:

$$\chi^{\rm dru} = \frac{-1}{M}\frac{\omega + i\varpi_D}{(\omega - \omega^{(1)})(\omega - \omega^{(2)})(\omega - \omega^{(3)})} \tag{B.12}$$

where $\omega^{(k)}$ are the solutions of (B.7).

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